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H, He, He^+ , Li^+ , and Mg^+ . The best approximation (A4) is then used for more complex atomic systems such as Li, C^{+3} , C^+ , N^+ , O^+ , O, Ne^+ , Na^+ , and K^+ . A4 generally agrees better with experiment than the Born or Coulomb-Born approximation. Exchange approximations (A5-A8) are characterized by different choices of asymptotic charges in the exchange amplitude. These approximations have been tested on hydrogen and although a slight improvement over the non-exchange approximations has been obtained in the case of A5, the difference does not appear to be too significant.

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ELECTRON IONIZATION CROSS SECTIONS IN
THE DISTORTED-WAVE APPROXIMATIONI. INTRODUCTION

The purpose of this report is to present results of distorted-wave (DW) calculations of electron impact ionization cross sections. Our investigation has been stimulated by the need for reliable cross section data for a large number of ions for which experimental results are not available, and by the inaccuracy of most theoretical methods which often overestimate the value of the ionization cross sections.

The accuracy of various approximations usually becomes better as the energy of incident electrons increases and therefore we have concentrated our study on the low-energy region where the reliability of different methods can be easily assessed. The exact quantum-mechanical evaluation of an ionization cross section is not possible because it would involve a prohibitively large volume of numerical calculations. Our goal was to develop an approximation based on the quantum-mechanical approach to the collision problem, simple enough so that it would be suitable for practical calculations, and such that it would give more reliable results than similar methods. We have investigated several modifications of the distorted-wave approximation which appear to be appropriate for this purpose.

In Section II we present an outline of the general theory of ionization for hydrogen and hydrogenic ions and in Section III we discuss approximate methods which will be used for comparison with our own results. The distorted-wave approximation without exchange is described in Section IV. We introduce four versions of the DW approximation which are characterized by different orthogonal properties of wave functions and by different choices of asymptotic charges for the ejected electron. Results of these

four modifications are compared for H, He, He^+ , Li^+ , and Mg^+ . The best approximation is then used for the calculation of ionization cross sections for more complex atoms. In Section V we study the effect of exchange on the ionization of hydrogen. Results are presented for four exchange approximations in which different choices of asymptotic charges were used in the exchange amplitude. The reliability of all approximations is discussed in Section VI.

II. GENERAL THEORY FOR HYDROGEN AND HYDROGENIC IONS

The total cross section for ionization is given by the expression¹⁻³

$$Q(E) = \frac{1}{2} \int_0^{E-E_i} \sigma(k_0, k, k') d\left(\frac{1}{2} k^2\right), \quad (1)$$

where $E = \frac{1}{2} k_0^2$ is the energy of the incident electron, E_i the ionization energy, \vec{k} and \vec{k}' are momenta of the two free electrons after an ionizing collision, and $\sigma(k_0, k, k')$ is the single differential cross section (SDCS) for ionization. All quantities in (1) and throughout this paper are expressed in atomic units except the cross section, which will be given in units of $\pi a_0^2 = 8.7974 \times 10^{-17} \text{ cm}^2$. Since the two electrons in the final state cannot be distinguished from each other,

$$\sigma(k_0, k, k') = \sigma(k_0, k', k) \quad (2)$$

and the integral in (1) is symmetric with respect to $\frac{1}{2} k^2 = \frac{1}{2} (E-E_i)$.

The integration can be cut off at $\frac{1}{2} (E-E_i)$ so that

$$Q(E) = \int_0^{\frac{1}{2}(E-E_i)} \sigma(k_0, k) d\left(\frac{1}{2} k^2\right) \quad (3)$$

with $\sigma(k_0, k) = \sigma(k_0, k, k')$ for $k \leq k'$.

SDCS for the ionization of the ground state of hydrogen and hydrogenic ions can be written in terms of scattering amplitudes in the form¹⁻³

$$\sigma(k_0, k, k') = \frac{k k'}{\pi k_0} \int \left\{ |f(\vec{k}, \vec{k}')|^2 + |g(\vec{k}, \vec{k}')|^2 - |f| |g| \cos(\beta - \beta') \right\} d\hat{k} d\hat{k}'. \quad (4)$$

$f(\vec{k}, \vec{k}')$ and $g(\vec{k}, \vec{k}')$ are the direct and the exchange scattering amplitude, respectively, \hat{k} and \hat{k}' are unit vectors in the direction of \vec{k} and \vec{k}' , and

$$\beta = \arg f, \quad \beta' = \arg g.$$

It has been shown by Peterkop⁴ that the direct and exchange amplitudes are related by

$$f(\vec{k}, \vec{k}') = g(\vec{k}', \vec{k}) \quad (5)$$

so that (2) is satisfied.

The integral expression for $f(\vec{k}, \vec{k}')$ is³

$$f(\vec{k}, \vec{k}') = - (2\pi)^{-\frac{5}{2}} \exp \left[i \Delta(\vec{k}, \vec{k}') \right] \quad (6)$$

$$\times \int \Psi(\vec{r}_1, \vec{r}_2) (H - E_{\text{total}}) \Phi(\vec{r}_1, \vec{r}_2) d\vec{r}_1 d\vec{r}_2.$$

$\Psi(\vec{r}_1, \vec{r}_2)$ is the exact unsymmetrized solution of the Schrödinger equation describing the scattering of the incident electron with the coordinate \vec{r}_2 on the atom with the bound electron which has the coordinate \vec{r}_1 . H is the total Hamiltonian, E_{total} is the energy of the system and $\Phi(\vec{r}_1, \vec{r}_2)$ is a function with asymptotic form

$$\phi(\vec{r}_1, \vec{r}_2) \sim \phi(z, -\vec{k}; \vec{r}_1) \phi(z', -\vec{k}'; \vec{r}_2), \quad (7)$$

where the functions ϕ satisfy equations of the form

$$\left[\nabla^2 + k^2 + \frac{2Z}{r} + 2V(r) \right] \phi(z, -\vec{k}; \vec{r}) = 0 \quad (8)$$

and asymptotically describe incident and scattered waves. The continuum functions ϕ are normalized per unit electron density at infinity. $V(r)$ may be any short-range potential and the effective charges Z and Z' are related by

$$\frac{Z}{k} + \frac{Z'}{k'} = \frac{Z_0}{k} + \frac{Z_0}{k'} - \frac{1}{|\vec{k} - \vec{k}'|} \quad (9)$$

with Z_0 equal to the residual charge of the atom or ion after ionization. Equation (9) follows from the condition that the scattering amplitude shall have no divergent phase factor. It has a simple classical interpretation: at large distances, $r_1 \sim k t$, $r_2 \sim k' t$, where t is the time, and consequently (9) can be written as

$$\frac{Z}{r_1} + \frac{Z'}{r_2} = \frac{Z_0}{r_1} + \frac{Z_0}{r_2} - \frac{1}{|\vec{r}_1 - \vec{r}_2|}.$$

The charges Z and Z' can therefore be interpreted as angle-dependent quantities which asymptotically take full account of the Coulomb potentials. The phase $\Delta(\vec{k}, \vec{k}')$ in (6) is given by

$$\Delta(\vec{k}, \vec{k}') = 2 \left[\frac{Z}{k} \ln \left(\frac{k}{X} \right) + \frac{Z'}{k'} \ln \left(\frac{k'}{X} \right) \right] \quad (10)$$

with $\frac{1}{2} X^2 = E - E_1$, provided that (9) is satisfied.

III. APPROXIMATE METHODS

Approximate methods for the evaluation of the scattering amplitude (6) must be used because the exact solution $\Psi(\vec{r}_1, \vec{r}_2)$ of the Schrödinger equation is not known. Moreover, it is difficult to satisfy condition (9) for effective charges Z and Z' as they depend on the angles between \vec{k} and \vec{k}' . If (9) is not satisfied, then the relative phases of the direct and exchange amplitude remain undetermined and have to be prescribed independently of any other approximation.

Approximation methods fall in two categories: non-exchange approximations in which the exchange amplitude gain (4) is neglected, and approximations where exchange is taken fully into account. Non-exchange approximations are computationally much simpler and may be successfully used for high energies of incident electrons, when exchange is relatively unimportant. The effect of exchange may sometimes be reduced by partial cancellation of the two terms in (4) containing g , which explains why the non-exchange approximations often give satisfactory results for complex atoms.

Our discussion of various approximate methods will be restricted to a few basic approximations which will be used later for comparison with our final results.

3.1 Non-exchange Approximations.

These approximations assume that $g = 0$ in equation (4). The value of the phase $\Delta(\vec{k}, \vec{k}')$ does not affect the result.

The simplest and most widely used method is the Born approximation for neutral atoms. For the ionization of hydrogen from the 1s state it adopts the conventions

$$Z = Z_0, \quad Z' = Z_0 - 1,$$

$$\Psi(\vec{r}_1, \vec{r}_2) = \psi(1s; \vec{r}_1) \exp(i\vec{k}_0 \cdot \vec{r}_2),$$

$$\Phi(\vec{r}_1, \vec{r}_2) = \varphi(Z_0, -\vec{k}; \vec{r}_1) \exp(-i\vec{k}' \cdot \vec{r}_2),$$

(11)

$$V(r) = 0.$$

In the Coulomb-Born (CB) approximation for hydrogenic ions with nuclear charge Z_0 , $\exp(i\vec{k}_0 \cdot \vec{r}_2)$ in (11) is replaced by $\varphi(Z_0-1, \vec{k}_0; \vec{r}_2)$ and $\exp(-i\vec{k}' \cdot \vec{r}_2)$ by $\varphi(Z', -\vec{k}'; \vec{r}_2)$.

In the non-exchange approximations, the two electrons in the final state are considered to be distinguishable and therefore (2) is not valid. Consequently the expression (1) for the total cross section is not identical to (3). Using (1) for the calculation of the total cross section, one has to omit the factor $\frac{1}{2}$ because it is associated with the indistinguishability of electrons. Then (1) together with (11) gives the Born (a) approximation (according to the notation introduced by Rudge³). On the other hand, equation (3) leads to the Born (b) approximation.

In the Born(a) method, the ejected electron (with the coordinate \vec{r}_1) is associated with the effective charge Z_0 for all values of the momentum k . This has an unsatisfactory consequence for $k > k'$, because the effective charge acting on the faster electron is larger than that acting on the slower one. A comparison of the Born(a) and Born(b) approximations for hydrogen is shown on Fig. 1. The Born(b) method usually gives substantially better results than the Born(a) approximation. Both the Born and the CB methods can be easily generalized to many-electron atoms and ions.

Many results from these approximations are now available^{1,14-20,42,44,45}. Various improvements have been attempted involving better approximations to Ψ and different choices of Z and Z' . The distortion of wave functions describing the free electrons in both the initial and final states can be taken into account by properly defining $V(r)$ in Eq. (8). Approximations with $V(r) \neq 0$ are usually referred to as distorted-wave (DW) approximations.

3.2 Exchange Approximations

The exchange amplitude $g(\vec{k}, \vec{k}')$ can be calculated from (5), and if Eq. (9) is not satisfied, the value of $\cos(\beta - \beta')$ has to be specified. By setting $\cos(\beta - \beta') = 0$ and using (11), we obtain an approximation which is identical to the Born(a) method. With the choice $\cos(\beta - \beta') = 1$ we get the Born-exchange approximation due to Peterkop⁵. This choice corresponds to maximum interference and therefore gives the smallest cross section of any approximation for the scattering amplitude. The Born-exchange approximation represents a substantial improvement in the calculated cross sections. It gives excellent agreement with experiment for the ionization of the ground state of He^+ , but for H it still overestimates the cross sections by about 30% at low energies (Fig. 3).

Another way to obtain the exchange amplitude is to use expression (6) for the direct amplitude and to replace $\Phi(\vec{r}_1, \vec{r}_2)$ by $\Phi(\vec{r}_2, \vec{r}_1)$. This procedure, together with the choice $\cos(\beta - \beta') = 1$ and Eq. (3) leads to the Born-Oppenheimer (BO) approximation. An attractive feature of this method is the possibility of deriving both the direct and exchange scattering amplitude from the expression analogous to (6) using

antisymmetric function Ψ and taking into account the spin of the electrons. In the BO approximation, (5) is satisfied if for $k > k'$ in the direct amplitude we define

$$\Phi(\vec{r}_1, \vec{r}_2) = \exp(-i\vec{k} \cdot \vec{r}_1) \varphi(Z_0, -\vec{k}'; \vec{r}_2). \quad (12)$$

Then Eq. (1) is identical to (3). As a consequence, the smaller effective charge is always associated with the faster of the two electrons, but the effective charges for individual electrons are discontinuous at $k = k'$. Another disadvantage of the BO method is the lack of orthogonality of Φ defined by (12) and Ψ given by (11). For the ionization of hydrogen, the BO approximation grossly overestimates cross sections at lower energies.¹⁴

The possibility of various choices of phases and effective charges associated with the direct and exchange amplitude leads to a large variety of approximations^{3,6,7,21-25}. However, for the ionization of hydrogen, no method has given results substantially better than the Born-exchange approximation.

IV. Ionization Cross Sections in the Non-Exchange DW Approximation

In this section we outline the approximation used in the present paper for the calculation of ionization cross sections without electron exchange. Four different approximations (A1 - A4) will be investigated and results will be presented for H, He, He^+ , Li^+ , and Mg^+ . Approximation A4 which appears to be most reliable will then be used for the calculation of ionization cross sections of more complex atomic systems.

4.1 General Description

In our approximation, distorted waves are used to describe the incident, scattered, and ejected electrons. For the ionization of hydrogen and hydrogenic ions we set

$$\Psi(\vec{r}_1, \vec{r}_2) = \psi(1s; \vec{r}_1) \varphi(Z_0 - 1, \vec{k}_0; \vec{r}_2), \quad (13)$$

$$\Phi(\vec{r}_1, \vec{r}_2) = \varphi(Z, -\vec{k}; \vec{r}_1) \varphi(Z', -\vec{k}'; \vec{r}_2). \quad (14)$$

The short-range potential $V(r)$ corresponding to φ describing the incident electrons in (13) represents an additional effect of nuclear charge and the screening of the bound electron. We put

$$V(r) = V_{1s}(r), \quad \text{with} \quad (15)$$

$$V_{1s}(r) = r^{-1} - r^{-1} \int_0^r \left[P(1s; x) \right]^2 dx + \int_r^\infty x^{-1} \left[P(1s; x) \right]^2 dx. \quad (16)$$

Leaving the choice of effective charges Z and Z' for the time being open, we define $V(r)$ corresponding to the functions φ in (14) by

$$V(r) = \theta(Z, Z_0) (Z_0 - Z) V_{1s}(r) \quad (17)$$

with a similar expression for Z' instead of Z . $\theta(Z, Z_0)$ is the step function given by

$$\theta(Z, Z_0) = 0 \text{ for } Z > Z_0, \theta(Z, Z_0) = 1 \text{ for } Z \leq Z_0. \quad (18)$$

Definition (17) formally guarantees a gradual change from the full screening by the bound electron to no screening if $Z_0 = Z$ or Z' .

Ionization cross sections are calculated from Eq. (3) and (4) with $g = 0$. We now generalize this approximation to complex atoms and ions. Let us consider a collision process in which an electron is ejected from the $n\ell_1^q$ shell. To obtain the expression for the single differential cross section σ , we have to sum over all possible final states of the ejected electron and over all final terms $n\ell_1^{q-1} S'L'$ of the remaining ion. Using partial wave expansions for the functions ϕ in (13) and (14) and assuming LS coupling, we obtain^{2,26}

$$\sigma(n\ell_1^q; k_0, k) = 16q k_0^{-2} \sum_{\lambda \ell \ell' \ell'_1} (2\lambda+1)^{-1} (2\ell+1) (2\ell'+1) (2\ell'_1+1) \times \begin{pmatrix} \ell & \ell' & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} \ell_1 & \ell'_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \left[R_\lambda^d(\ell_1 \ell; \ell'_1 \ell') \right]^2 \quad (19)$$

where ℓ_1, ℓ, ℓ'_1 and ℓ' are angular momentum quantum numbers of the bound, incident, ejected (slower), and scattered (faster) electron, respectively. Parameter λ corresponds to the multipole order in the expansion for the interaction potential. The direct radial integral is given by

$$R_\lambda^d(\ell_1 \ell; \ell'_1 \ell') = \int P(n\ell_1; r_1) F(Z_0-1, k_0, \ell; r_2) \left[\delta(\lambda, 0) U(r_1) + \delta(\lambda, 0) U'(r_2) + \frac{r_1^\lambda}{r_2^{\lambda+1}} \right] F(Z, k, \ell'_1; r_1) F(Z', k', \ell'; r_2) dr_1 dr_2 \quad (20)$$

with

$$U(r_1) = (Z - Z_0) \left[r_1^{-2} + \theta(Z, Z_0) v_{n\ell_1}(r_1) \right], \quad (21)$$

$$U'(r_2) = (Z' - Z_0) \left[r_2^{-2} + \theta(Z', Z_0) V_{nl_1}(r_2) \right]. \quad (22)$$

$P(nl_1; r)$ is the radial function of the bound electron in the nl_1 orbit and the continuum functions $F(a, b, c; r)$ are solutions of

$$\left[\frac{d^2}{dr^2} - \frac{c(c+1)}{r^2} + \frac{2a}{r} + 2V(r) + b^2 \right] F(a, b, c; r) = 0 \quad (23)$$

normalized so that at infinity

$$F(a, b, c; r) \sim b^{-1/2} \sin \left[br + ab^{-1} \ln(2cr) + \eta \right]. \quad (24)$$

$V_{nl_1}(r)$ is given by (16) if $P(1s; x)$ is replaced by $P(nl_1; x)$. For complex atoms we set

$$V(r) = V_c(r) + \theta(A, Z_0) (Z_0 - A) V_{nl_1}(r), \quad (25)$$

where Z_0 is the residual charge of the ion after ionization, A is equal to Z or Z' for the continuum functions of the final state and to $Z_0 - 1$ for the initial state, $\theta(A, Z_0)$ is defined by (18), and

$$V_c(r) = Nr^{-1} - \sum_{i=1}^N \left\{ r^{-1} \int_0^r \left[P_i(x) \right]^2 dx + \int_r^\infty x^{-1} \left[P_i(x) \right]^2 dx \right\}. \quad (26)$$

The summation in (26) is carried out over all bound electrons in the final state described by radial functions P_i . In this procedure we take into account only the spherical component of the interaction potential in calculating the distortion of continuum wave functions.

Unlike in the Born(b) and CB(b) methods, the wave functions of the initial and final state of the total system with distorted continuum

functions representing free electrons are generally not orthogonal. In our DW approximation, the orthogonality is achieved by solving Eq. (23) for $F(Z, k, \ell'_1; r_1)$ with the right-hand side replaced by $\epsilon_1 P(n\ell_1; r_1)$ if $\ell'_1 = \ell_1$. Parameter ϵ_1 is adjusted so that $\int P(n\ell_1; r) F(Z, k, \ell_1; r) dr = 0$. Then expression (21) for $U(r_1)$ will contain an additional term

$$-\epsilon_1 P(n\ell_1; r_1), \quad (27)$$

but radial integrals (20) will not depend on $U'(r_2)$ due to the orthogonality of $P(n\ell_1; r)$ and $F(Z, k, \ell_1; r)$.

If the initial or final state of the system is represented by an antisymmetric function, the procedure described above is not sufficient to assure orthogonality. This may be achieved by orthogonalizing also the continuum function $F(Z', k', \ell'; r)$ of the scattered (faster) electron to $P(n\ell_1; r)$. Although such an additional orthogonalization is not required by necessity in non-exchange approximations, it may change the computed cross sections and we will investigate its effects in the following sections. We will also introduce two different choices of effective charge Z , thus having four approximations, A1 - A4.

4.2 Approximation A1.

In order to keep our calculations as simple as possible, we will assume that charges Z and Z' are independent of the angles between \vec{k} and \vec{k}' . This automatically implies that Eq. (9) will not be satisfied and we must use other considerations to determine their values.

First of all, the violation of condition (9) may not be as serious as it appears, because in the calculation of scattering amplitudes

according to (6), the most important parts of the φ functions are those close to the atom. In this region, the form of φ is predominantly determined by all possible interactions of atomic and free electrons, of which only some were taken into account by the form of $V(r)$ in (8). By a proper adjustment of Z and Z' one may include effects of other neglected interactions and achieve a better representation of the functions φ in this important region, even if (9) is not satisfied.

Secondly, Eq. (9) is not sufficient by itself to determine uniquely both Z and Z' , and if Z' is arbitrarily chosen, then (9) may lead to a physically unsatisfactory value of Z . For example, if we choose $Z' = 0$ for neutral atoms and if both electrons move in the same direction, then from (9) $Z = 1 + \frac{k}{k'} - \frac{k}{k'-k} < 1$ and therefore the corresponding φ will describe the slower electron as being subject to the force $-Z r_1^{-2} > -r_1^{-2}$, while actually it is subject to the force $-r_1^{-2} - (r_2 - r_1)^{-2} < -r_1^{-2}$.

In the Born and the CB approximations it is assumed that the full residual charge Z_0 is acting on the slower electron in the final state. Eq. (9) then takes the form

$$Z' = Z_0 - k' |\vec{k} - \vec{k}'|^{-1} \quad (28)$$

and the choice $Z' = Z_0 - 1$ is compatible with the spherical average of (28) over all directions of \vec{k} .

In the AI approximation we adopt the same choice of Z and Z' and set

$$Z = Z_0, \quad Z' = Z_0 - 1. \quad (29)$$

Due to the value of Z' , the continuum functions $F(Z', k', \ell'; r_2)$ for the scattered electron are orthogonal to $F(Z_0 - 1, k_0, \ell; r_2)$ and therefore the radial integrals (20) are independent of $U(r_1)$ given by (21) and (27).

4.3 Approximation A2

The choice of Z and Z' is the same as in A1, but we use continuum functions $F(Z', k', \ell'; r)$ orthogonalized to $P(n\ell_1; r)$ if $\ell' = \ell_1$. This procedure introduces an additional term

$$- \epsilon_2 P(n\ell_1; r_2) \quad (30)$$

into the expression (22) for $U'(r_2)$, but that does not affect radial integrals (20) as they do not depend on $U'(r_2)$. On the other hand, the radial integral with $\ell = \ell' = \ell_1 = \ell_1'$ will now contain a non-vanishing contribution corresponding to $U(r_1)$ due to the lack of orthogonality of $F(Z_0 - 1, k_0, \ell; r_2)$ and $F(Z', k', \ell'; r_2)$. This contribution is presumably small and will be ignored in the present approximation.

4.4 Approximation A3

In considering the choice of Z and Z' for the direct scattering amplitude, we start from the experimental observation that, for incident energies not far above the threshold, the double differential cross section (DDCS) for ionization is larger for scattering angles $\vartheta < 90^\circ$ than for $\vartheta > 90^\circ$. This applies to both the faster and the slower electrons. For the faster electrons, the DDCS has a strong peak in the forward direction, while the DDCS for slower electrons shows a much less pronounced maximum around $\vartheta = 60^\circ$. This can be interpreted as a manifestation of the fact that both electrons move predominantly in the forward direction, especially when they are close together, before their mutual repulsion increases the angle between their velocities. Therefore, instead of taking a spherical average of $|\vec{k} - \vec{k}'|$ in (9), we determine Z and Z' by assuming that \vec{k} is parallel to \vec{k}' . The effective charges may be interpreted in

several ways and we obtain various conditions for Z and Z' :

- (a) In accordance with (9) and our assumption about \vec{k} and \vec{k}' , we get

$$\frac{Z}{r_1} + \frac{Z'}{r_2} = \frac{Z_0}{r_1} + \frac{Z_0}{r_2} - \frac{1}{r_2 - r_1}, \quad (31)$$

using $r_1 \sim kt$, $r_2 \sim k't$.

- (b) If we require the actual force acting on the slower electron to be $-\frac{Z}{r_1^2}$, we obtain

$$-\frac{Z}{r_1^2} = -\frac{Z_0}{r_1^2} - \frac{1}{(r_2 - r_1)^2}. \quad (32)$$

- (c) The same condition written for the faster electron is

$$-\frac{Z'}{r_2^2} = -\frac{Z_0}{r_2^2} + \frac{1}{(r_2 - r_1)^2}. \quad (33)$$

- (d) Classically both electrons move in such a way that the force acting on the center of gravity is equal to $-\frac{Z_0}{r_1^2} - \frac{Z_0}{r_2^2}$. We may require the same force to act on the center of gravity if the electrons are moving in the field of effective charges Z and Z' and we obtain

$$-\frac{Z}{r_1^2} - \frac{Z'}{r_2^2} = -\frac{Z_0}{r_1^2} - \frac{Z_0}{r_2^2}. \quad (34)$$

All four conditions are simultaneously satisfied if Z and Z' are chosen according to (32) and (33). For $r_1/r_2 \rightarrow 0$ we obtain

$$Z \sim Z_0 + (r_1/r_2)^2, \quad Z' \sim Z_0 - 1 - (r_1/r_2)^2. \quad (35)$$

However, our basic assumption about the parallelism of \vec{k} and \vec{k}' cannot be valid in the limit of $r_1/r_2 \rightarrow 1$, and conditions (31) - (33) are not applicable. On the other hand, Eq. (34) does not contain the term $(r_2 - r_1)^{-1}$ and is therefore more appropriate for the determination of Z and Z' in the limit of $r_1/r_2 = 1$. Generally, if \vec{k} is not parallel to \vec{k}' , the radial component of the force acting on the center of gravity of the two electrons is equal to $-\frac{Z_0}{2} \cos \alpha - \frac{Z_0}{2} \cos \beta$, where α and β are angles between the direction to the center of gravity and the vectors \vec{k} and \vec{k}' , respectively. If the effective charges produce the same force, then,

$$-\frac{Z}{r_1} \cos \alpha - \frac{Z'}{r_2} \cos \beta = -\frac{Z_0}{r_1} \cos \alpha - \frac{Z_0}{r_2} \cos \beta. \quad (36)$$

For small values of r_1/r_2 , (36) is equivalent to (34) due to the assumption of parallelism between \vec{k} and \vec{k}' . When $r_1/r_2 \rightarrow 1$, α approaches β regardless of the angle between \vec{k} and \vec{k}' and in the limit again (36) becomes equivalent to (34). Therefore Eq. (34) is approximately satisfied for all values of r_1/r_2 . Thus we adopt the following expression for Z :

$$Z = Z_0 \left[1 + \left(\frac{r_1}{r_2} \right)^2 \right] - Z' \left(\frac{r_1}{r_2} \right)^2. \quad (37)$$

If the scattering amplitude is calculated from (6) using functions (13) and (14), it is much less sensitive to the value of Z' (associated with the faster electron) than to Z . In order to simplify the calculations, we therefore adopt a constant value of Z' and define

$$Z' = Z_0 = 1 \quad (38)$$

in agreement with (35) in the limit of $r_1/r_2 = 0$. This choice is consistent with the Born and CB methods and with our approximations A1 and A2.

Putting $r_1/r_2 \sim k/k'$, Eq. (37) together with (38) gives finally

$$Z = Z_0 + (k/k')^2. \quad (39)$$

Eq. (39) agrees with (35) which is valid for small values of k/k' . According to this choice, the attractive force acting on the slower electron is larger than the force caused by the residual charge of the ion. As a result, it is more difficult for the ejected electron to escape and this leads to the lowering of the ionization cross section. An unsatisfactory property of the choice (38) and (39) is that in the limit of $k = k'$ the effective charges of the two electrons differ by 2. Moreover, the assumption that both electrons move predominantly in the forward direction is of questionable validity near the threshold of ionization.

Similarly to the A1 approximation, the continuum functions for the incident and scattered electrons are orthogonal and all terms in radial integrals associated with $U(r_1)$ and $U'(r_2)$ vanish.

4.5 Approximation A4

The choice of Z and Z' is the same as in A3 and is given by (38) and (39). In A4, continuum functions $F(Z', k', \ell'; r)$ with $\ell' = \ell_1$ are orthogonalized to $P(n\ell_1; r)$ as in A2 and resulting additional terms in the radial integral associated with $U(r_1)$ are ignored.

Basic characteristics of approximations A1 - A4 together with the Born and CB methods are summarized in Table 1.

Table 1

Approximation	Z	Z'	V(r)	Function of the Scattered (slower) Electron
Born and CB	Z_0	$Z_0 - 1$	0	Orthogonal to $P(nl_1; r)$
A1	Z_0	$Z_0 - 1$	$\neq 0$	
A2	Z_0	$Z_0 - 1$	$\neq 0$	
A3	$Z_0 + (k/k')^2$	$Z_0 - 1$	$\neq 0$	
A4	$Z_0 + (k/k')^2$	$Z_0 - 1$	$\neq 0$	

4.6 Results and Discussion

In the numerical evaluation of (19) we have included the first five angular momenta l_1' corresponding to the ejected (slower) electron. That was found sufficient in most cases in the low-energy region with $E/E_1 \leq 4$. The summation over l and l' has been carried out until convergence has been reached. The number of angular momenta taken into account was usually less than 20. For each value of $E = \frac{1}{2} k_0^2$ we have computed $\sigma(k_0, k)$ for 4 values of k . Hartree-Fock wave functions of bound electrons calculated by Clementi and Roetti²⁹ have been used for non-hydrogenic atomic systems.

The differences between various approximations diminish as the incident electron energy increases. At the same time the number of angular momenta l and l' which should be taken into account becomes

prohibitively large. Therefore we have made calculations in the low-energy region, where the reliability of different methods can be easily assessed.

Results from approximations A1 - A4 for H, He^+ , He, Li^+ , and Mg^+ are shown in Table 2. In Figs. 1 - 5 they are compared with experimental data and with other approximations. Two general conclusions can be drawn from Table 2: Firstly, the use of continuum functions for the scattered (slower) electron orthogonalized to the bound wave function (approximations A2 and A4) always reduces the value of the cross section, and secondly, the choice of effective charge Z given by (39) in A3 and A4 has the same effect. The differences are most pronounced in the low-energy region as expected, and the effect of orthogonalization is much smaller for ions than for neutral atoms. Approximation A4 yields the lowest cross sections and appears to be the best in comparison with experiment.

For hydrogen (Fig. 1), A1 and A2 give results similar to the Born(b) approximation except near the threshold. Approximations A3 and A4 lead to a substantial improvement of results, especially in the energy region where the cross section reaches its maximum value. Very close to the threshold, A4 appears to underestimate the cross sections for H and He. However, in the case of hydrogen, the value 0.076 for $E/E_1 = 1.25$ represents the lower limit, because omitted contributions from $\ell_1' > 4$ in (19) may not be negligible. Measurements for hydrogen represented by curves 3 and 4 in Fig. 1 were normalized to the Born approximation at high energy. If these measurements were normalized to absolute data of Rothe et al.¹¹ shown by curve 5, the maximum value of the cross section would be reduced

by about $0.1 \pi a_0^2$. As a result, even the A4 approximation would still slightly overestimate the cross section in the maximum region, but the agreement in the low-energy region would be improved.

Approximations A3 and A4 agree very well with experimental data for He^+ at all energies (Fig. 2). For the Helium-like systems (Figs. 3 and 4) there is a discrepancy in the region of maximum cross section. A4 overestimates the value of Q by about 20% and the difference is probably due to the omission of exchange, which is known to reduce substantially excitation cross sections in helium-like ions³².

For Mg^+ , A1 and A2 give very large cross sections compared to experiment and also to the CB(b) approximation (Fig. 5). A possible explanation for this difference may be the focusing effect of the short-range potential $V(r)$ on incident electrons in the DW approximation. This effect may be compensated in A3 and A4 by a larger attractive force acting on the ejected electron so that a good agreement with experimental data is achieved.

In Table 3 we present ionization cross sections calculated in approximation A4 for several atoms and ions of increasing complexity. The results for two representative energies are compared with experiment and with other theoretical methods. For atoms and ions with ground configurations consisting of several terms we have used ionization energies which correspond to the lowest term. It was also assumed that all final terms have the same energy in agreement with the derivation of Eq. (19). Effects of autoionization have been neglected and the cross sections for atoms with the $ns^2 np^q$ configurations have been evaluated from both the ns^2 and np^q subshells.

The approximation A4 gives smaller ionization cross sections than the Coulomb-Born method for almost all ions shown in Table 3 and generally agrees better with experiment. The theoretical cross sections computed in A4 for C^+ , N^+ , and O^+ at $E/E_i = 4$ are in a good agreement with measured values. High experimental cross sections in the low-energy region with $E/E_i = 2$ for these ions are most likely to be attributed to the effect of autoionization of metastable levels which are populated by excitation of the 2s electron. This effect has been discussed by Moores.¹⁶ In the case of ions with closed or almost closed up shells (Ne^+ , Na^+ , K^+), A4 overestimates the cross sections by about 25%, but the results for K^+ agree with measurements of Peart and Dolder.⁴³ The worst agreement is obtained for C^{+3} , where the values shown in Table 3 represent a lower limit due to the omission of terms with $\lambda_1' > 4$. It is interesting to note that no other approximation was able to reproduce the experimental results for this ion, although the agreement for the next isoelectronic ion, N^{+4} , was found satisfactory.⁴⁰ Theoretical cross sections for neutral oxygen are in satisfactory agreement with experiment regarding the uncertainty of measured data.

We conclude that the approximation A4 is the best of all four non-exchange approximations A1 - A4, and it generally yields better results than the Born(b) or Coulomb-Born(b) method except, perhaps, in the low-energy region close to the ionization threshold, where it may underestimate the cross sections.

V. EFFECT OF EXCHANGE IN THE DW APPROXIMATION

5.1 General Considerations

In the following sections we will investigate the effect of exchange scattering amplitude $g(\vec{k}, \vec{k}')$ on the value of ionization cross sections and our discussion will be restricted to the ground state ionization of hydrogen.

The total cross section for ionization is calculated from (3) and (4) and the exchange scattering amplitude is obtained from the direct amplitude by employing relation (5). According to Eq. (3), $k \leq k'$. We adopt the convention that effective charge Z is always associated with momentum k , i.e. with the slower electron in the final state.

Expanding the continuum functions into partial waves we obtain for the ionization of $H(1s)$

$$\begin{aligned} \sigma(k_o, k) = 16 k_o^{-2} \sum_{\ell \ell' \ell'_1} (2\ell+1) (2\ell'+1) (2\ell'_1+1) \begin{pmatrix} \ell & \ell' & \ell'_1 \\ 0 & 0 & 0 \end{pmatrix}^2 \\ \times \left\{ \left[R_{\ell'_1}^d(\ell_1 \ell; \ell'_1 \ell') \right]^2 + \left[(2\ell'+1)^{-1} (2\ell'_1+1) R_{\ell'}^e(\ell_1 \ell; \ell'_1 \ell') \right]^2 \right. \\ \left. - (2\ell'+1)^{-1} (2\ell'_1+1) |R_{\ell'_1}^d(\ell_1 \ell; \ell'_1 \ell')| |R_{\ell'}^e(\ell_1 \ell; \ell'_1 \ell')| \cos(\gamma - \gamma') \right\}. \end{aligned} \quad (40)$$

Direct radial integrals R_λ^d are given by (20) and exchange integrals R_λ^e are defined by

$$R_{\lambda}^e(\ell_1 \ell; \ell'_1 \ell') = \int P(1s; r_1) F(Z_0 - 1, k_0, \ell; r_2) \left[\delta(\lambda, 0) U(r_2) + \delta(\lambda, 0) U'(r_1) + \frac{r_{<}^{\lambda}}{r_{>}^{\lambda+1}} \right] F(Z, k, \ell'_1; r_2) F(Z', k', \ell'; r_1) dr_1 dr_2. \quad (41)$$

The value of $\gamma - \gamma'$ is associated with relative phases of the direct and exchange part of the element of the scattering matrix which connects channels characterized by k_0, ℓ and k, ℓ'_1, k', ℓ' . Our choice of Z and Z' does not satisfy condition (9) and therefore there is no point in attempting to determine $\gamma - \gamma'$ from Eq. (10). In our approximation we set

$$\cos(\gamma - \gamma') = 1$$

in analogy to the choice of relative phases in the Born-exchange approximation⁵. Expression (40) is valid also for ionization of hydrogen and hydrogenic ions from any ns state if $P(1s; r)$ in (41) is replaced by $P(ns; r)$, and for ionization of atoms with one ns electron outside closed shells if $V(r)$ is properly defined according to (25) and (26).

The results of non-exchange DW approximations presented in Section 4.6 indicate that the approximation A4 gives the best overall agreement with experiment. We therefore adopt the same choice of Z and Z' as in A4 for the calculation of direct integrals in (40), i.e.

$$Z = Z_0 + (k/k')^2, \quad Z' = Z_0 - 1. \quad (42)$$

Moreover, in agreement with A4 we orthogonalize both continuum functions $F(Z, k, \ell'_1; r)$ and $F(Z', k', \ell'; r)$ with $\ell'_1 = 0$ and $\ell' = 0$ to the bound function $P(1s; r)$ as described in section 4.1. The orthogonalization of

continuum functions appearing in the exchange integral is performed as well. Due to the orthogonal property of $P(ls; r)$ and $F(Z', k', l'; r)$, the contribution to the integral (41) associated with $U(r_2)$ vanishes.

According to Eq. (5) the exchange amplitude $g(\vec{k}, \vec{k}')$ with $k < k'$ is equal to the direct scattering amplitude for the process in which the ejected electron has a higher velocity than the scattered one. The direct amplitude may be interpreted on the basis of a classical picture of the scattering process and one can see that the effective charges Z and Z' in the case when the ejected electron is faster need not necessarily be associated with the charges Z and Z' when it is slower. Therefore, even if Z and Z' were specified by (42) for direct radial integrals, we have to determine their values separately for exchange integrals. We will investigate four different choices described in the following sections.

5.2 Approximation A5

In the expression for exchange radial integrals we put

$$Z = Z_0 - 1, \quad Z' = Z_0 + (k/k')^2. \quad (43)$$

This choice is analogous to the effective charges adopted in the Born-exchange approximation in the sense that the exchange amplitude can be obtained from the direct amplitude by interchanging \vec{k} and \vec{k}' in (14). If the exchange amplitude is interpreted as a direct amplitude according to (5), then effective charges for both electrons are continuous at $k = k'$. This is shown graphically on Fig. 6, where effective charges are plotted against k/k' (with $k \leq k'$) in such a way that the diagram

covers the whole interval of possible velocities of the ejected electron.

With respect to the choice of Z , the integral

$$\int F(Z_0 - 1, k_0, \ell; r) F(Z, k, \ell'_1; r) dr$$

is either zero or has a small value so that the contribution to R_λ^e corresponding to $U'(r_1)$ may be neglected. An unsatisfactory property of the choice (43) is associated with the fact that the charge for the slower electron in the exchange amplitude is smaller than the charge acting on the faster electron, a situation which is similar to the Born-exchange approximation.

5.3 Approximation A6

In this approximation, the exchange amplitude is obtained from the direct amplitude by interchanging \vec{r}_1 and \vec{r}_2 in (14) as in the Born-Oppenheimer approximation. This procedure leads to the choice

$$Z = Z_0 + (k/k')^2, \quad Z' = Z_0 - 1 \quad (44)$$

for effective charges in (41). The higher charge is always associated with the slower of the two electrons, but the charges are discontinuous at $k = k'$ (Fig. 6).

The functions $F(Z_0 - 1, k_0, \ell; r)$ and $F(Z, k, \ell'_1; r)$ with $\ell = \ell'_1$ are not orthogonal because $Z \neq Z_0 - 1$ and consequently the contribution to the exchange integral corresponding to $U'(r_1)$ does not vanish. Nevertheless, we will ignore this contribution in the present approximation.

5.4 Approximation A7

In analogy to our assumption about the parallelism of \vec{k} and \vec{k}' in the direct amplitude, we will assume that, if the ejected electron has a higher velocity, the vectors \vec{k} and \vec{k}' are antiparallel. In the classical model it means that the ejected electron moves in the forward direction, while the scattered electron moves backwards. This assumption takes explicitly into account the possibility of the backscattering which is well documented by experimental evidence. Using the same arguments as in Sec. 4.4, we define

$$Z = Z_0 - (k/k')^2, \quad Z' = Z_0 - 1 \quad (45)$$

in the exchange amplitude.

In this approximation, the charge for electron with coordinate \vec{r}_2 is continuous at $k = k'$ (Fig. 6) and the slower of both electrons is always associated with a higher effective charge. An unsatisfactory consequence of (45) is that it leads to full screening of both electrons at $k = k'$. As in A6, we will ignore the non-vanishing contributions to R_λ^e associated with $U'(r_1)$ in (41).

5.5 Approximation A8

With the choice

$$Z = Z' = Z_0 \quad (46)$$

adopted in this approximation for exchange amplitude, $U'(r_1)$ vanishes according to (22) and effective charges are discontinuous at $k = k'$ (Fig. 6). This choice is similar to the one used by Geltman and Hidalgo²² in the Coulomb-projected Born approximation.

Various characteristics of exchange approximations A5 - A8 are summarized in Table 4.

5.6 Results and Discussion

Results from approximations A5 - A8 for the ground state ionization of hydrogen are shown in Table 5 and Fig. 7, where they are compared with experiment, the Born-exchange method and the non-exchange approximation A4.

The symbol $>$ indicates that the number of angular momenta l_1' included in the calculation was not sufficient and therefore the value shown in the table represents a lower limit. Approximation A5 gives the lowest cross sections and the best agreement with experimental data if one takes into account the possibility that a different normalization according to absolute measurements of Rothe et al.¹¹ would lower curve 2 in Fig. 7. However, A5 underestimates cross sections near the threshold, where better results are obtained from A7. Approximation A6 gives very unsatisfactory results for all energies in spite of its theoretical attractiveness. Compared to the non-exchange approximation A4, only A5 gives lower cross sections at all energies, but the difference is not too pronounced and it is smaller than the difference between the Born(b) and Born-exchange approximations.

The differences between various approximations are more conspicuous if one compares the partial contributions to the single differential cross section $\sigma(k_0, k)$. Table 6 shows a typical example for one incident energy $E = 2E_1$. The dominant contribution at low k^2 corresponds to $l_1' = 1$ in all approximations. With increasing k^2 the contributions from

higher values of l_1' become more important, notably in A6, A7 and A8. The importance of exchange increases with increasing k^2 and the differences between various approximations are most significant in the limit $k = k'$. They also increase with decreasing energy E . This is shown on Figs. 8 - 10 which represent the single differential cross section $\sigma(k_0, k)$ for three energies of incident electrons. The effects of exchange are least pronounced in A5 and one can see why the total cross sections in this approximation are little different from the non-exchange approximation A4: the decrease of σ caused by exchange at low values of k^2 is partially compensated by an increase for k^2 approaching $E - E_1$.

VI. SUMMARY AND CONCLUSION

In the present investigation we have studied eight different modifications of the distorted-wave approximation for the calculation of electron ionization cross sections. From the non-exchange approximations A1 - A4, A4 appears to be the most satisfactory and generally gives a better agreement with experiment than the Born or Coulomb-Born approximations, without excessive requirements on the computing time. It is therefore suitable for a production of large number of data needed in the analysis and interpretation of hot plasmas in laboratory devices and in astronomical objects.

Exchange approximations A5 - A8 have been tested on hydrogen, and A5 has been found superior to A6 - A8. Ionization cross sections obtained in A5 are slightly lower than those from A4, but the difference does not appear to be too significant with respect to the uncertainty of experimental data used for comparison. The small effect of exchange in the A5

approximation may be just a particular property of hydrogen, but good agreement of the non-exchange approximation A4 with measured cross sections in many other cases suggests more general validity of this property.

For incident energies corresponding to $E/E_i > 4$, the importance of exchange rapidly decreases and in this region A4 is expected to give reliable cross sections for all atoms and ions.

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Table 2

Ionization Cross Sections (in πa_0^2) in the Non-Exchange DW Approximation

Atom	Approximation	E/E_i			
		1.25	2	4	10
H(1s)	A1	0.401	0.815	1.012	0.629
	A2	0.112	0.672	0.994	0.629
	A3	0.291	0.594	0.771	
	A4	> 0.076	0.499	0.759	0.535
He ⁺ (1s)	A1	0.0230	0.0577	0.0644	0.0394
	A2	0.0207	0.0563	0.0644	0.0394
	A3	0.0194	0.0487	0.0563	
	A4	0.0173	0.0474	0.0563	
He(1s ²)	A1	0.115	0.379	0.556	
	A2	0.045	0.326	0.548	
	A3	0.120	0.326	0.475	
	A4	0.040	0.283	0.469	
Li ⁺ (1s ²)	A1	0.0191	0.0541	0.0661	
	A2	0.0172	0.0509	0.0659	
	A3	0.0174	0.0484	0.0597	
	A4	0.0156	0.0471	0.0586	
Mg ⁺ (3s)	A1	0.421	0.788	0.650	
	A2	0.406	0.782	0.649	
	A3	0.279	0.562	0.566	
	A4	0.269	0.556	0.566	

Table 3

Comparison of the Non-Exchange DW Method (Approximation A4) with Other
Methods and With Experiment. Ionization Cross Sections Given in Units πa_0^2 .

Method		E/E _i	
		2	4
Li(2s)	A4	3.170	3.600
C ⁺ (2s)	A4	>0.0340	> 0.0340
	CB(b) ³⁹	0.036	0.036
	Exp. ¹²	0.024	0.026
C ⁺ (2s ² 2p)	A4	0.393	0.588
	CB(b) ¹⁶	0.491	0.676
	Exp. ⁴⁰	0.541	0.612
N ⁺ (2s ² 2p ²)	A4	0.370	0.582
	CB(b) ¹⁶	0.491	0.673
	Exp. ³⁶	0.42	0.58
O ⁺ (2s ² 2p ³)	A4	0.313	0.524
	CB(b) ¹⁶	0.439	0.609
	Exp. ¹³	0.377	0.498
O(2s ² 2p ⁴)	A4	0.586	1.524
	Born ⁴¹	0.745	1.1380
	Exp. ³⁷	0.682	1.36
	Exp. ³⁸		1.7
Ne ⁺ (2s ² 2p ⁵)	A4	0.236	0.440
	CB(b) ¹⁶	0.310	0.458
	Exp. ³⁵	0.190	0.345
Na ⁺ (2s ² 2p ⁶)	A4	0.192	0.370
	CB(b) ¹⁶	0.285	0.430
	Exp. ³⁴	0.160	0.295
K ⁺ (3s ² 3p ⁶)	A4	1.070	1.130
	CB(b) ⁴²	0.97	1.75
	Exp. ³⁴	0.88	0.96
	Exp. ⁴³	1.02	1.09

TABLE 4

Approximation	Effective Charge in the Exchange Amplitude		Effective Charge for the slower Electron is Higher	Term in (41) Associated with $U'(r_1)$ is small or vanishes	Effective Charges for Both Electrons are Continuous at $k = k'$
	Z (slower electron)	Z' (faster electron)			
A5	$Z_0 - 1$	$Z_0 + (k/k')^2$	No	Yes	Yes
A6	$Z_0 + (k/k')^2$	$Z_0 - 1$	Yes	No	No
A7	$Z_0 - (k/k')^2$	$Z_0 - 1$	Yes	No	No
A8	Z_0	Z_0	No	Yes	No

TABLE 5

Ionization Cross Sections (in πa_0^2) for Hydrogen

in the DW-Exchange Approximation

Approximation		E/E_i	
	1.25	2.0	4.0
A5	0.072	0.453	0.669
A6	> 0.245	> 0.898	> 0.820
A7	0.143	0.602	0.724
A8	0.340	0.575	0.673

TABLE 6

Partial Contributions to $k_0^2 \sigma(k_0, k)$ from angular momenta ℓ_1' of the

Slower Electron for $E/E_i = 2$. Ionization of H(1s)

Approximation	k^2	ℓ_1'				
		0	1	2	3	4
A4	0	1.021	7.783	1.228	0.0636	0.0014
	0.1667	0.352	3.217	1.185	0.193	0.1176
	0.3333	0.0485	0.979	0.780	0.260	0.0459
	0.5	0.0415	0.112	0.346	0.234	0.0738
A5	0	1.021	7.783	1.228	0.0636	0.0014
	0.1667	0.270	2.559	1.022	0.172	0.0158
	0.3333	0.0934	0.885	0.625	0.213	0.0379
	0.5	0.0661	0.475	0.385	0.212	0.0661
A6	0	1.088	6.672	1.384	0.113	0.0044
	0.1667	0.471	3.058	1.202	1.933	0.0172
	0.3333	0.380	1.546	2.451	1.643	0.671
	0.5	0.432	0.679	1.843	2.600	2.030
A7	0	1.088	6.672	1.384	0.113	0.0044
	0.1667	0.525	3.300	1.329	0.259	0.0355
	0.3333	0.413	1.929	0.956	0.304	0.0706
	0.5	0.303	0.882	0.440	0.221	0.0741
A8	0	1.060	6.161	1.071	0.0622	0.0018
	0.1667	0.492	2.711	1.148	0.210	0.0251
	0.3333	0.327	1.513	1.125	0.390	0.0886
	0.5	0.437	1.635	1.358	0.668	0.229

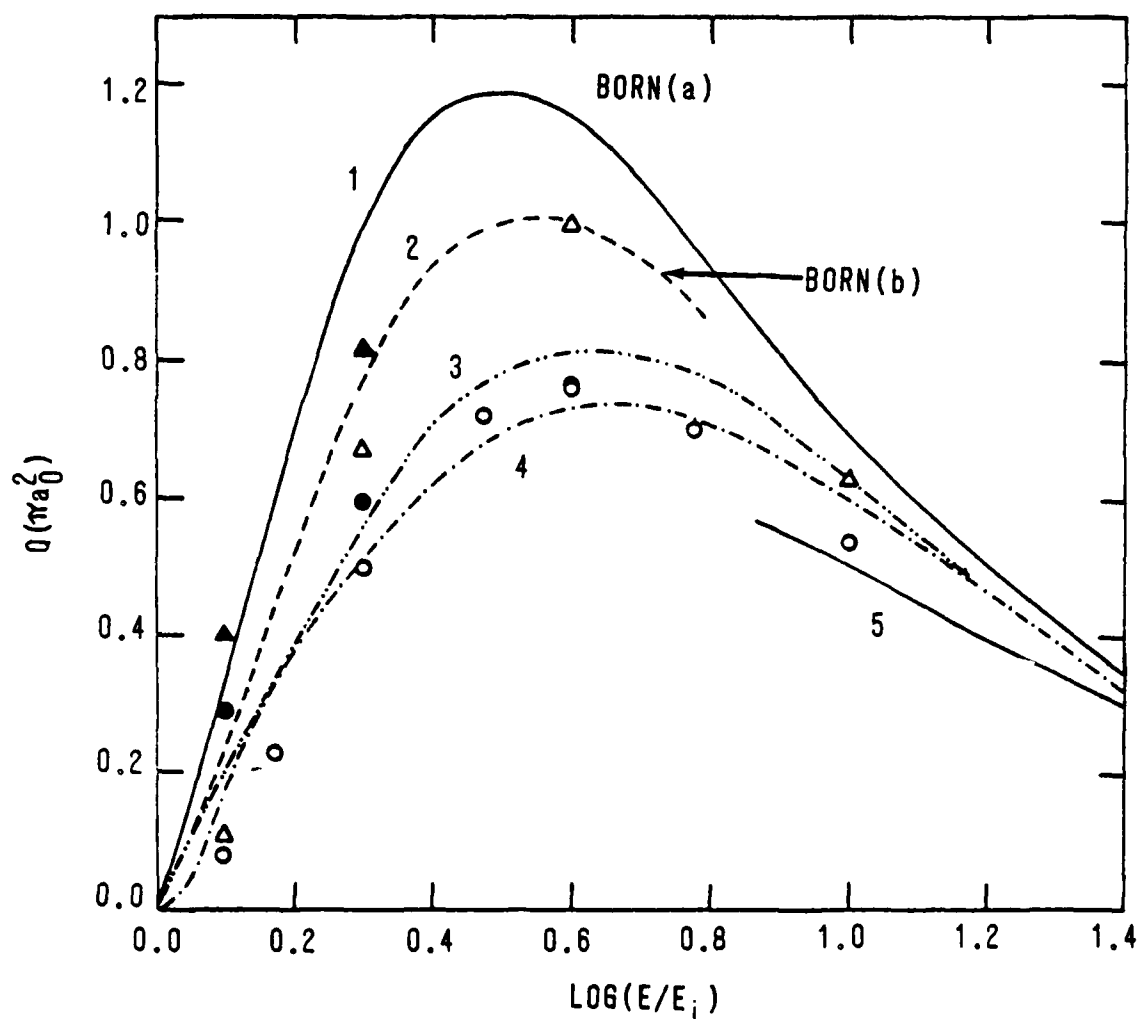


Fig. 1 — Cross sections for the ground state ionization of hydrogen. 1 — Born (a)¹; 3 — measurement of Fite and Brackmann⁸; 4 — measurement of Boksenberg^{9,10}; 5 — measurement of Rothe et al.¹¹; Δ — A1; \triangle — A2; \bullet — A3; \circ — A4.

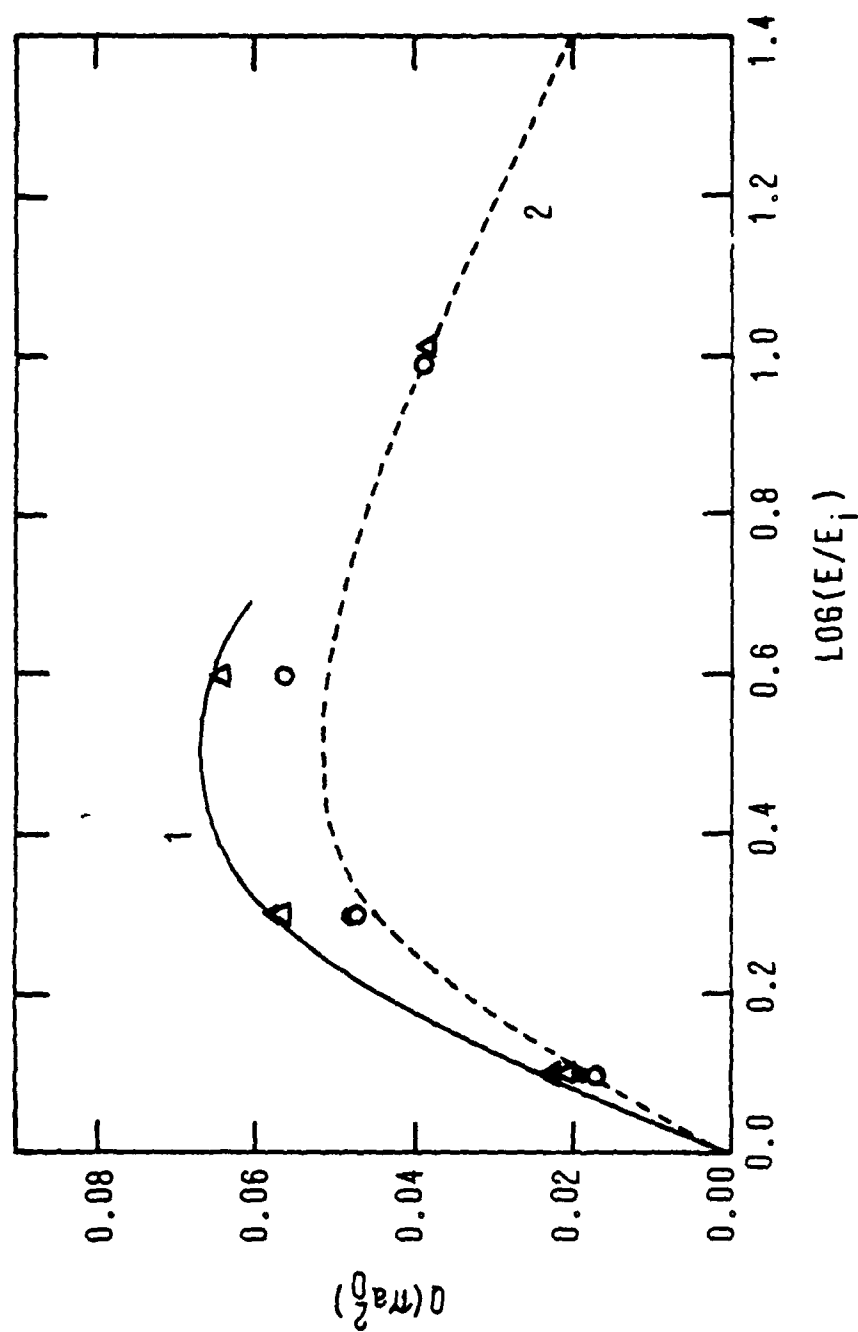


Fig. 2 — Cross sections for ionization of $\text{He}^+(1s)$. 1 — Coulomb-Born (b)²;
2 — measurement of Peart et al.³⁰; other symbols as for Fig. 1.

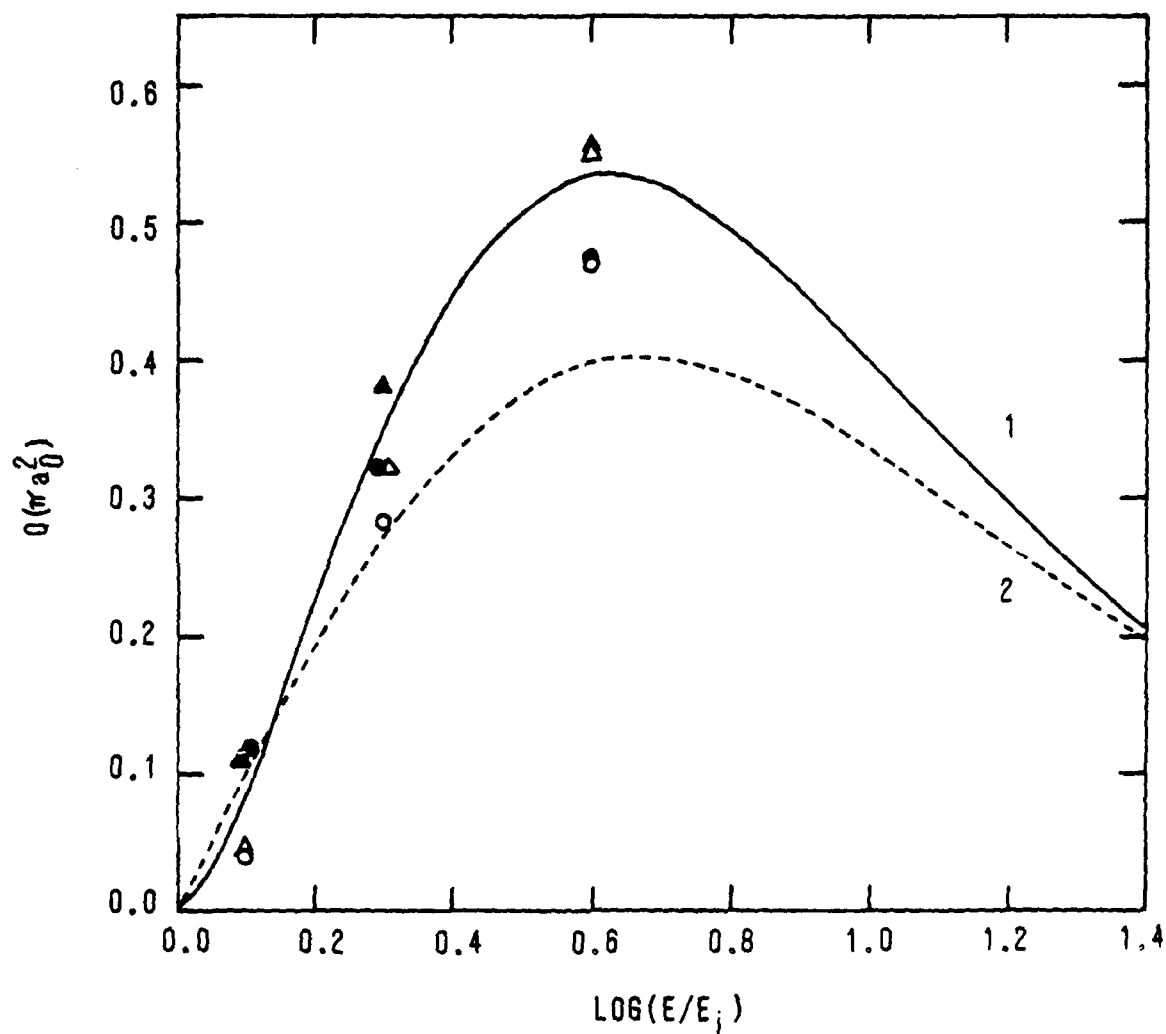


Fig. 3 — Cross sections for ionization of $\text{He}(1s^2)$. 1 — Born (b)²⁷; 2 — measurement of Smith²⁸; other symbols as for Fig. 1.

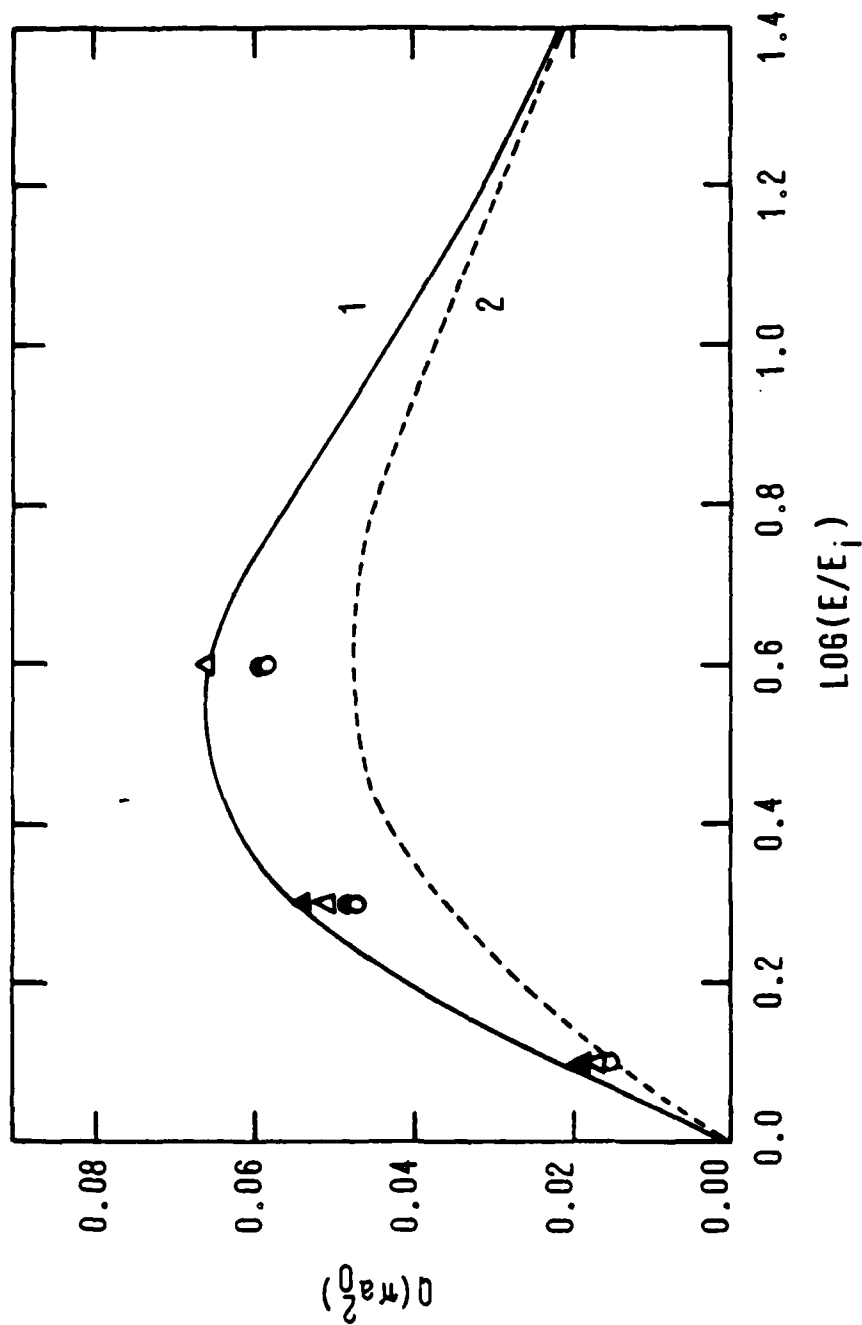


Fig. 4 — Cross sections for ionization of $\text{Li}^+(1s^2)$. 1 — Coulomb-Born (b)¹⁵;
2 — measurement of Peart and Dolder³³; other symbols as for Fig. 1.

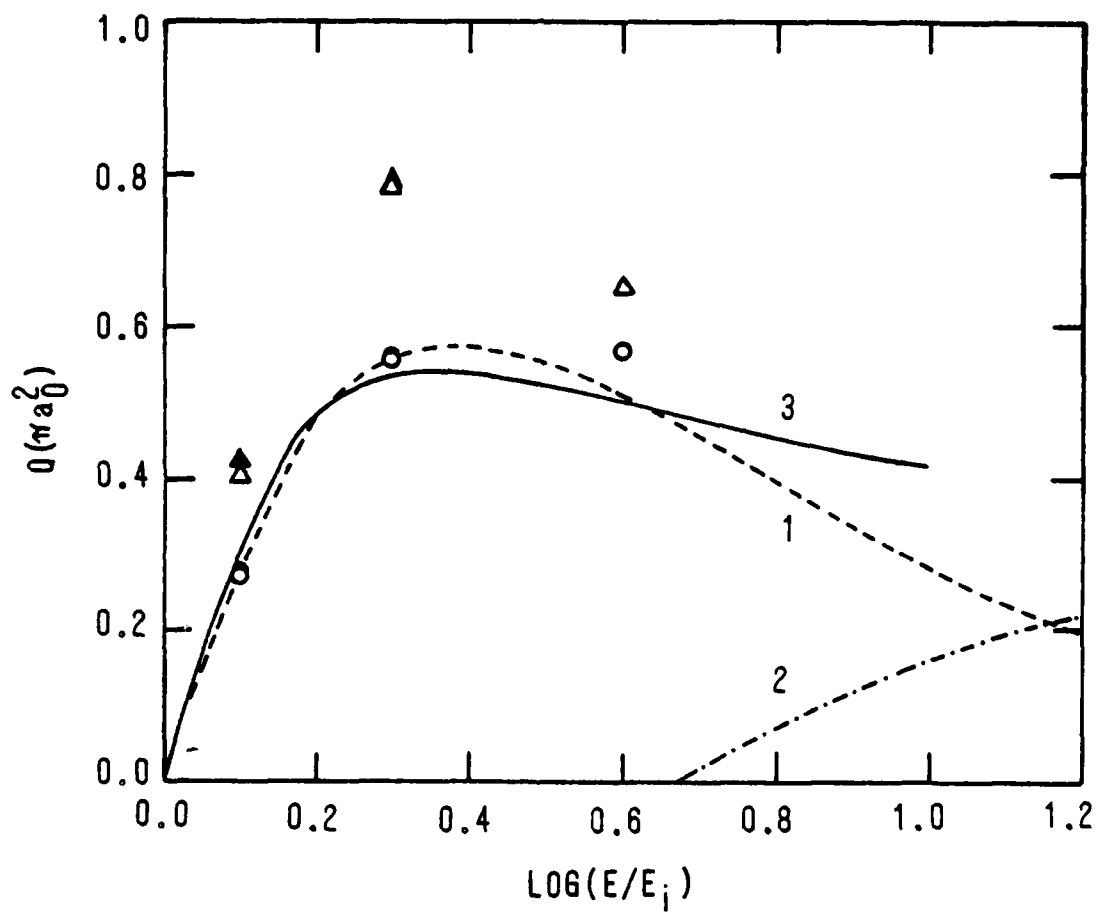


Fig. 5 — Cross sections for ionization of $\text{Mg}^+(3s)$. 1 — Coulomb-Born (b)¹⁵, ejection of 3s electron; 2 — Coulomb-Born (b)¹⁵; ejection of 2p electron; 3 — measurement of Martin et al.³¹, other symbols as for Figure 1.

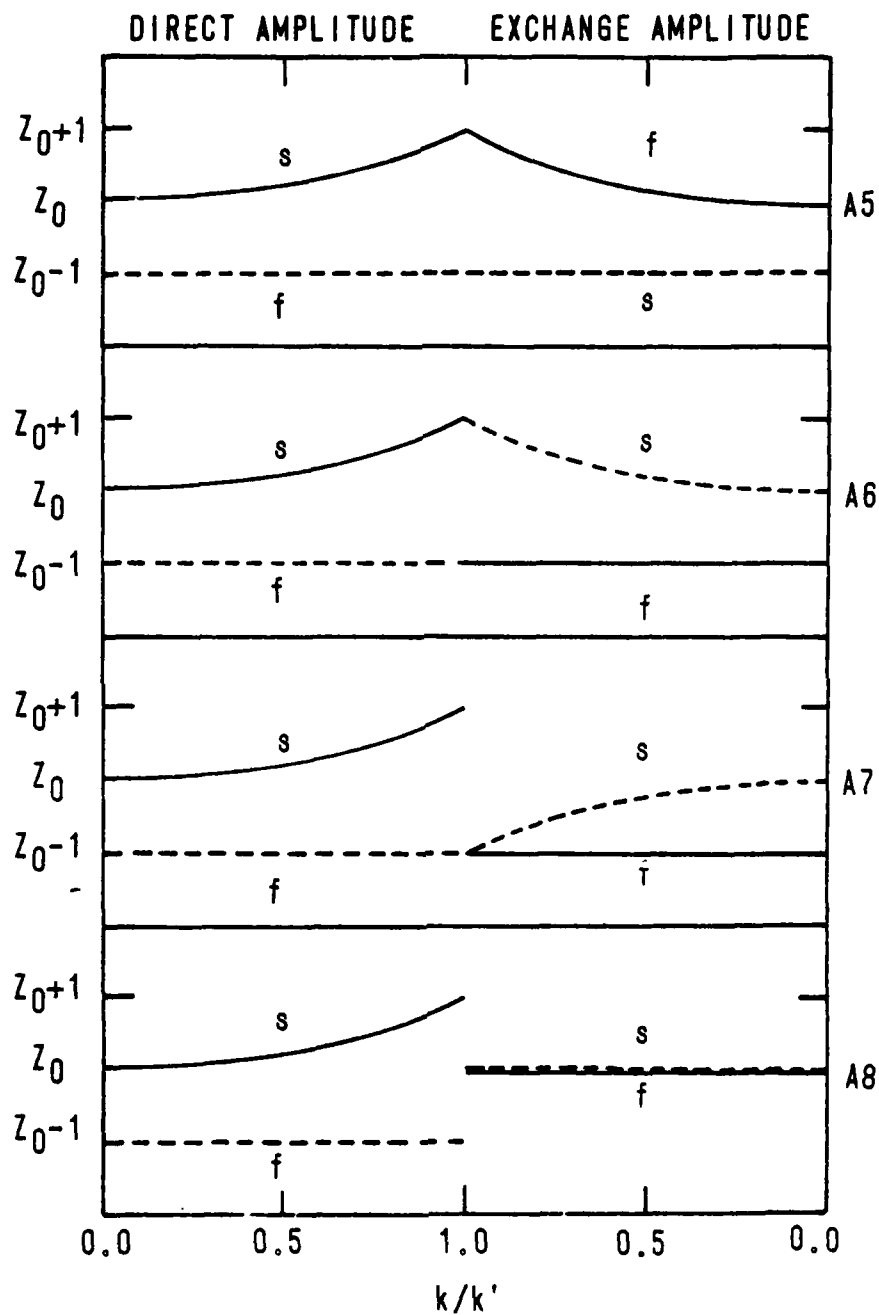


Fig. 6 — Effective charges acting on electron 1 (full line) and 2 (broken line) in approximations A5-A8. s — slower electron (charge Z), f — faster electron (charge Z')

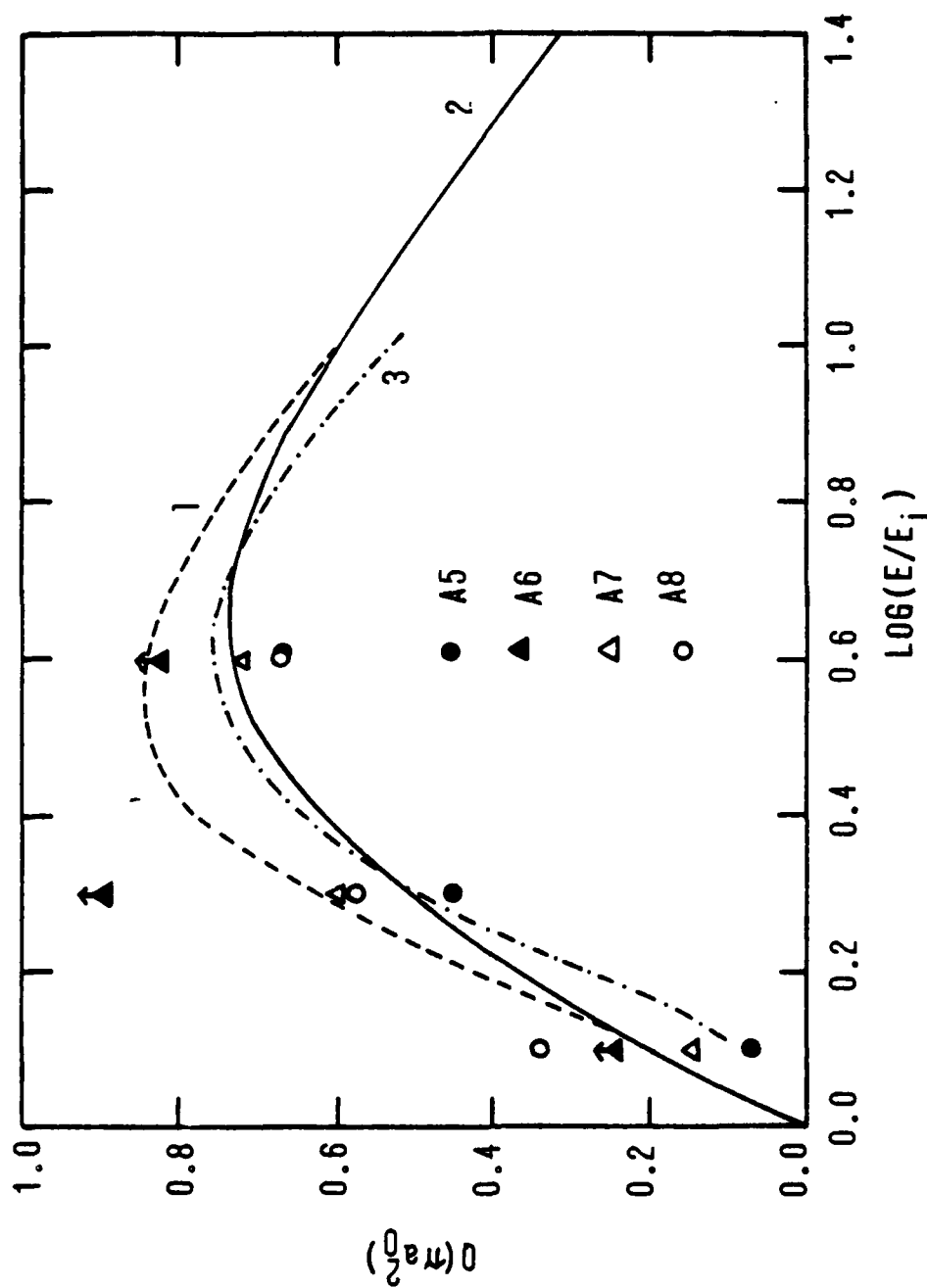


Fig. 7 — Cross sections for the ground state ionization of hydrogen. 1 — Born exchange^{1,5};
2 — measurement of Boksenberg^{9,10}; 3 — A4

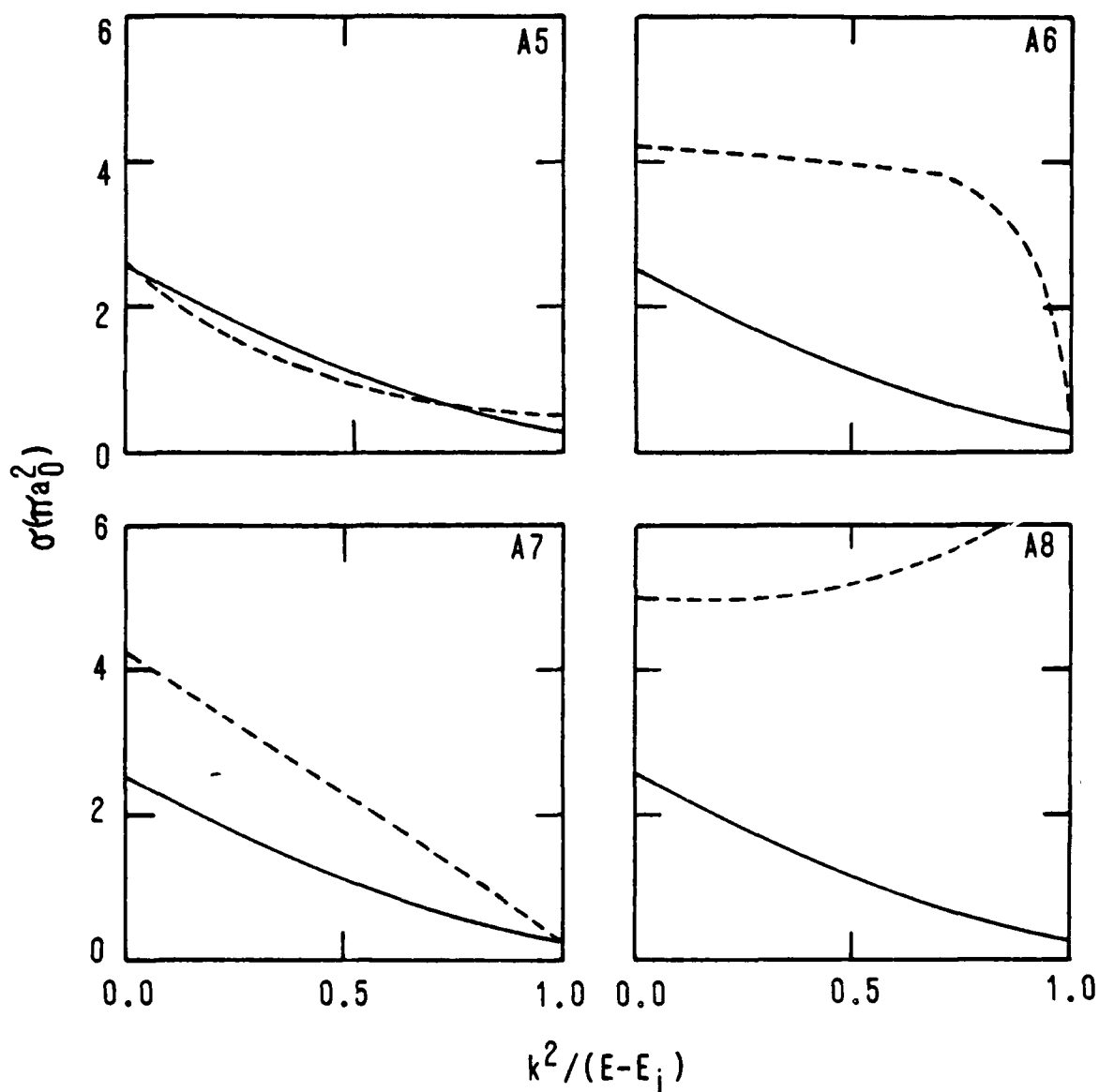


Fig. 8 — Single differential cross section $\sigma(k_0, k)$ for hydrogen. $E/E_i = 1.25$. Full line — A4; broken lines — exchange approximations A5- A8. Omitted terms in A4 and A6 would increase σ for k^2 close to $E - E_i$.

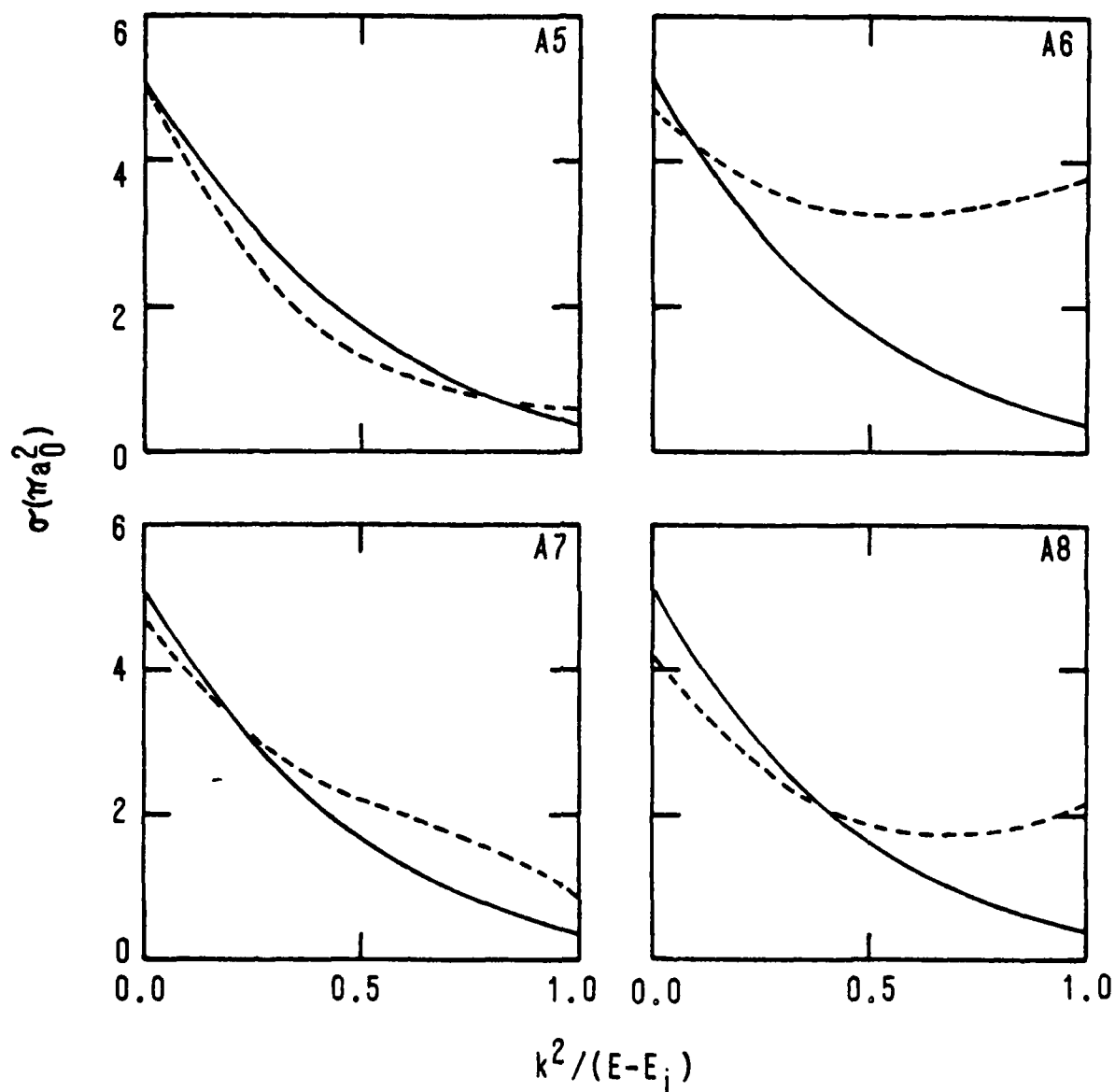


Fig. 9 — Same as Fig. 8. $E/E_i = 2$. Omitted terms in A6 would increase σ for k^2 close to $E - E_i$.

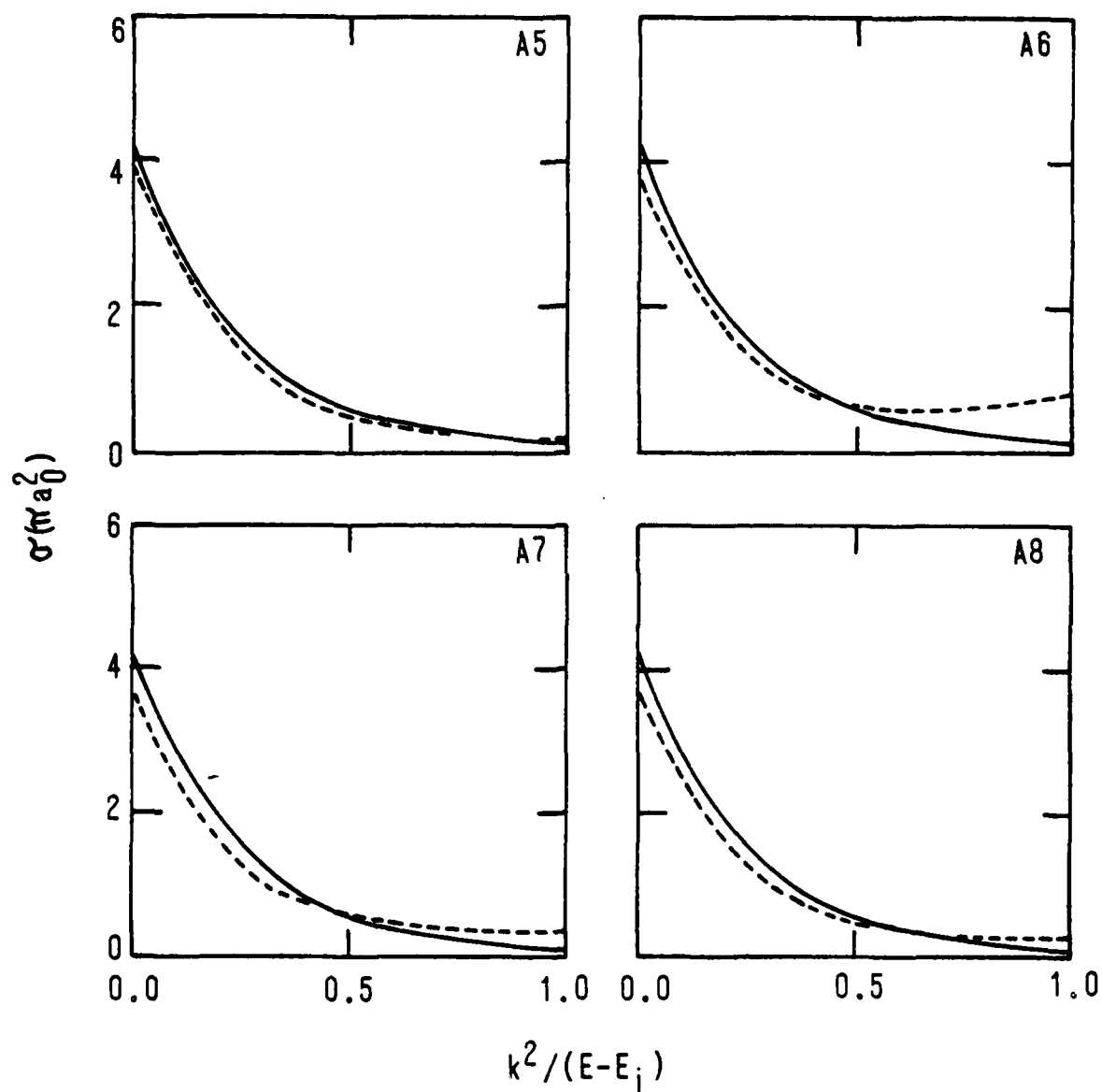


Fig. 10 — Same as Fig. 8. $E/E_i = 4$. Omitted terms in A6 would increase σ for k^2 close to $E - E_i$.